

Assessing the Mixing Performance of Extruders: Indices and Scale-up

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Abstract. This work proposes the use of global quantitative dispersive and distributive mixing indices to characterize the performance of a given screw. Calculation of these quantities uses a model of morphology evolution as a function of material and flow characteristics, which was coupled to a description of the flow developing along the screw from hopper to die. Scale-up on the basis of these indices is briefly discussed. Some results are presented in order to illustrate the usefulness of the methodology.

1- INTRODUCTION

Single screw extruders are deceptively simple machines, as their relatively uncomplicated construction hides the fact that they submit the material being processed to a complex thermo-mechanical environment. In fact, extruders are generally required to pump a homogeneous melt at the highest possible rate, which implies efficient solids conveying, melting and melt conveying, as well as adequate distributive and dispersive mixing of all ingredients (typically, polymer(s) and additives).

Mixing rate and intensity depend on several material characteristics, on operating conditions and on screw geometry [1-3]. Process engineers have been using their considerable creativity and skills to design screws that yield globally good mixing levels [4]. However, in industrial practice it remains difficult to predict how a given screw will perform in terms of mixing of a particular material, or to estimate/compare the mixing performance of various candidate screws.

This work attempts to define and use global quantitative (dispersive and distributive) mixing indices able to characterize the performance of a given screw (working under certain operating conditions). For example, when processing a system consisting of an immiscible polymer blend, or of a suspension of liquid/molten additives in an homopolymer, dispersion is related to the decrease (or increase, via coalescence) in size of the dispersed phase, whilst distribution can be estimated from the deformation of these drops. Therefore, global mixing indices can be determined from the overall changes in morphology suffered by the polymer system from its melting onset to the moment it exits the screw. Calculation of these quantities requires the development of a model of morphology evolution as a function of material and flow characteristics, which is then coupled to a description of the flow developing along the screw from hopper to die, under specific operating conditions and screw geometry.

If a given screw is performing well, namely from the mixing point of view, one may wish

to design a bigger (or smaller) screw retaining the same characteristics, i.e., one may wish to scale-up the process. Although a detailed explanation of scale-up methodologies lies beyond the framework of this text [5, 6], some results will be shown for scaling-up for mixing, using the mixing indices proposed.

2- MIXING MODEL

When two immiscible polymer melts, or a polymer and an additive, are mixed, a two-phase morphology is generated, the major component being the matrix and the other the dispersed phase, consisting of individual drops. Upon flow in the screw channel, break up and/or coalescence of these drops may occur (Figure 1), the first depending on the viscosity ratio between disperse phase and matrix, on the capillary number (relative intensity of viscous forces and surface tension) and on residence time [1], while coalescence depends on the probabilities of two drops colliding and expelling the film of polymer between them [7].

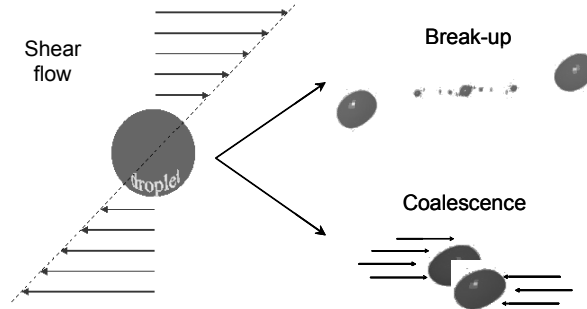


Figure 1: Drop break-up and coalescence

The dispersive mixing efficiency may be estimated, at any location, from the average change in drop size. Thus, if d and d_0 are the current and initial drop diameter, respectively, the following index can be used [8]:

$$mix_{disp} = \frac{\sum_j^N \left[\left(\frac{d}{d_0} \right)_j \times \left(1 - \frac{d}{d_0} \right)_j \right]}{\sum_j^N \left(\frac{d}{d_0} \right)_j} \quad (1)$$

where j is the total number of particles in the system. The computation of distributive mixing uses the concept of affine deformation of a drop, which is determined by shear rate and residence time [1]. The corresponding index is defined as:

$$mix_{dist} = \frac{\sum_j^N \left[\left(\frac{d}{d_0} \right)_j \times \left(1 - \frac{B}{d_0} \right)_j \right]}{\sum_j^N \left(\frac{d}{d_0} \right)_j} \quad (2)$$

where B and d are the drop width and diameter, respectively [8]. Both indices range between 0 and 1, higher values indicating better mixing. Figure 2 shows the sequence of calculations involved, a detailed description being given elsewhere [9].

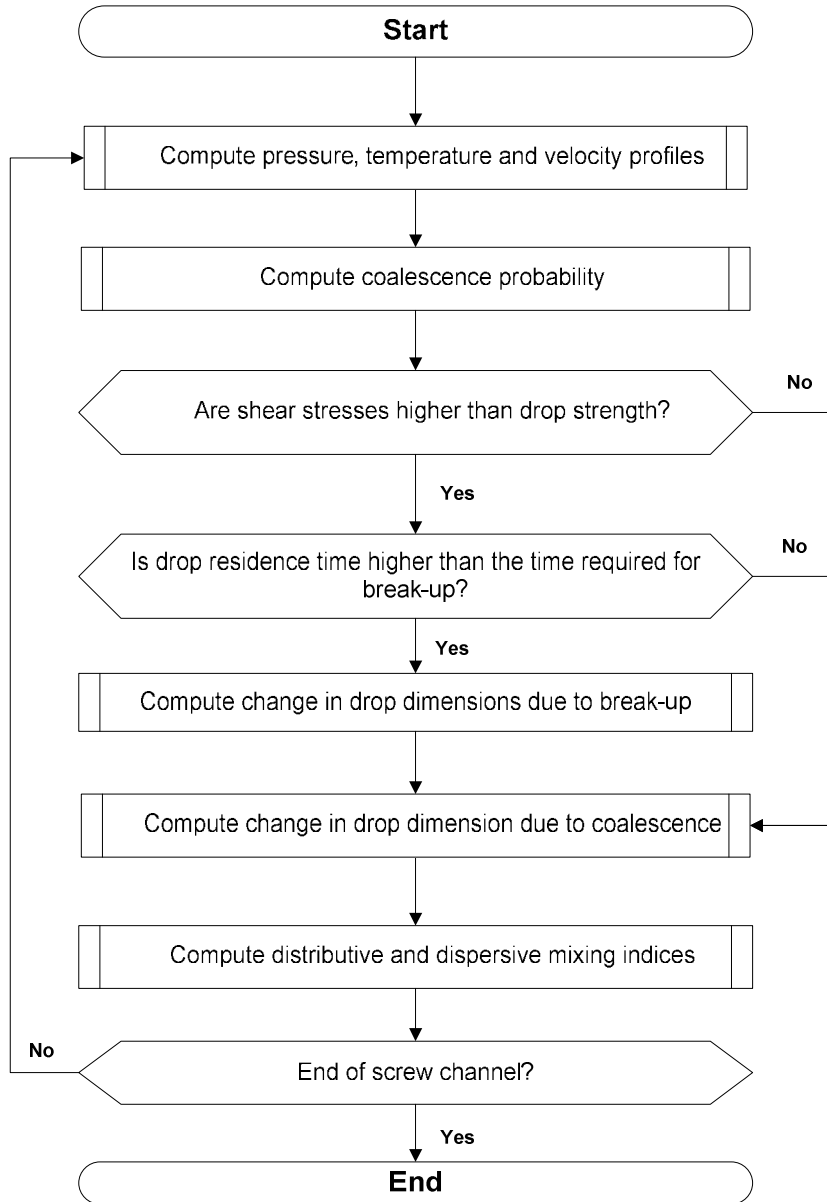


Figure 2: Calculation of the mixing indices

3- SCALE-UP METHODOLOGY

The aim of extrusion scale-up is to define the geometry and/or operating conditions of a target extruder, in order to subject the material being processed to the same flow and heat transfer conditions existing in the reference extruder, thus yielding products with the same characteristics. Various individual criteria (such as average shear rate, melting rate, or mixing) can be used in order to perform scale-up using simple analytical correlations [5, 6]. The authors have developed a methodology capable of dealing simultaneously with various criteria and of using the more precise predicting capabilities of numerical process modelling [10].

Scale-up is dealt with as a multi-objective optimization problem, where the various criteria are taken into consideration simultaneously and we seek to determine the geometry/operating conditions of the target extruder that minimize the differences in performance in relation to the reference extruder. More details about this methodology can be found elsewhere [10].

4- RESULTS AND DISCUSSION

As an example, a single screw extruder with a screw diameter of 30mm and $L/D = 30$ is considered. A commercial HDPE grade was selected as the polymer matrix. For computational purposes, a total of circa 10.000 drops with a radius of 10 μm were inserted as soon as melting is initiated and as uniformly distributed in the melt pool, in a quantity proportional to the amount of molten polymer in each cross section in the downchannel direction. The viscosity ratio between these drops and HDPE was taken as 1. The barrel temperature was set to 200°C.

Figure 3 compares the effect of screw speed on the mixing performance of two screws having the same diameter D , L/D and compression ratio, but feed and metering zones with different lengths (these are identified in the y-axis of Figures 3a and 3b). Figures 3a and 3b show that in both screws melting is initiated roughly at the same channel location, but a shorter feed zone is much more efficient for melting, as it brings on faster the more effective contribution of the compression zone (relative increase of the channel width to depth ratio, with more efficient heat transfer). While in Figure 3a melting may occupy a significant part of the metering zone, especially for the higher screw speed range, Figure 3b (longer metering section) shows a metering zone almost fully dedicated to melt conveying. These disparities trigger other distinct responses between the two screws, such as variations in average shear rates and residence times – affecting directly morphology development – due to distinct mass output (see Figures 3c and 3d, respectively). Figure 3e and 3f present the differences in terms of distributive and dispersive mixing performance, respectively. As expected, a longer metering zone induces better mixing, although the relative efficiency depends on the screw speed range, due to the complex influence of the latter on the various process parameters.

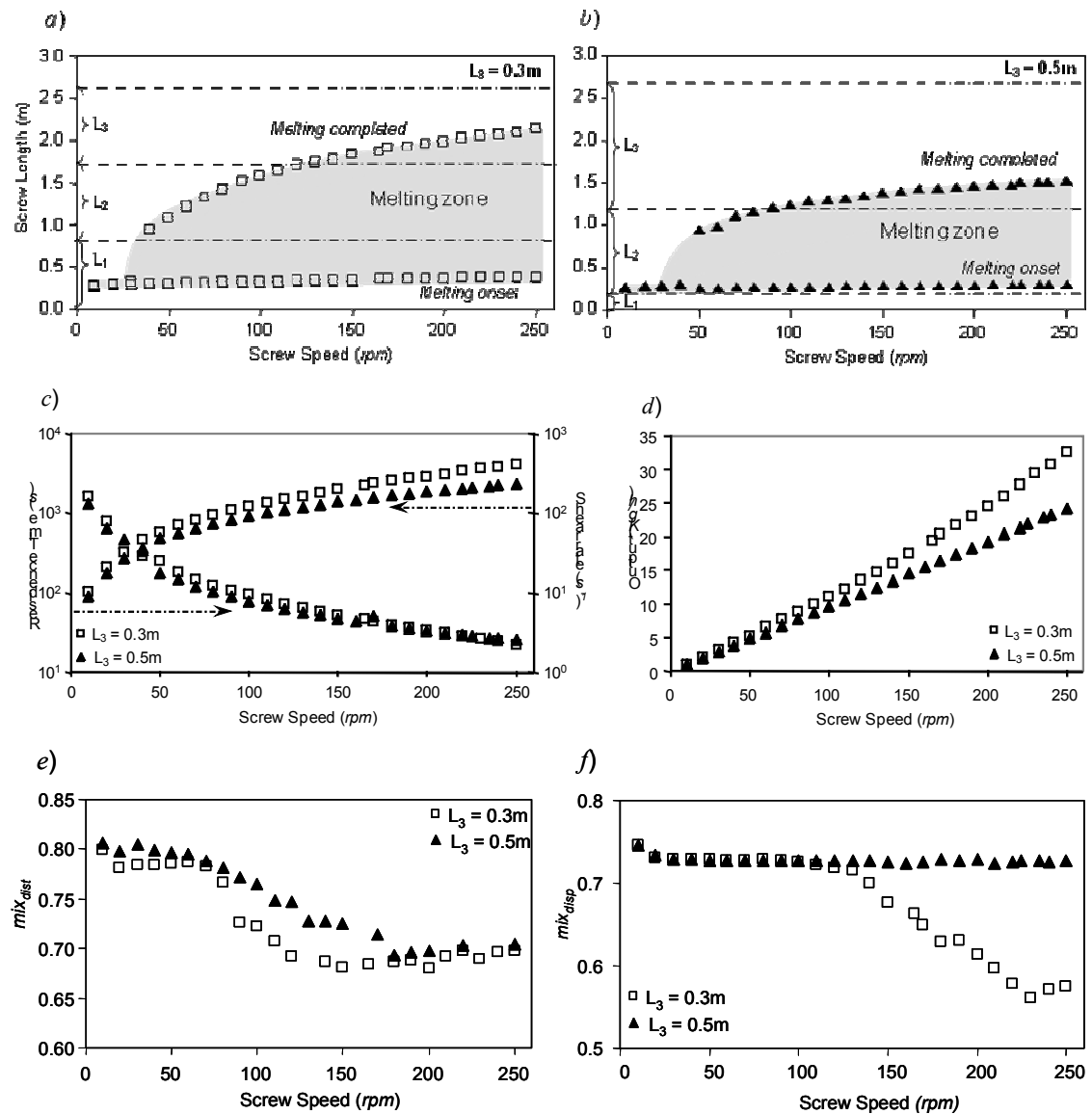


Figure 3: Effect of screw speed on the response of two screws with the same size but having feed and metering zones with different lengths. *a)* melting behaviour of screw with shorter metering; *b)* melting behaviour of screw with longer metering; *c)* average shear rate and residence time; *d)* mass output; *e)* global distributive mixing index; *f)* global dispersive mixing index.

Figure 4 shows the results of computations evidencing the effect of compression ratio on mixing. Compression ratio was modified by changing the channel depth at the feed section from 3 to 7 mm. The melting behaviour of the two screws is somewhat surprising, since the shallower screw takes longer to fully melt the material. This is due to the fact that, although radial conduction is less effective for higher screw depths, convection in the flow direction becomes smaller for the shallower screw, given the higher solid bed

average velocity (this assertion can be quantified via the Peclet number, which decreases twofold for the two compression ratios considered).

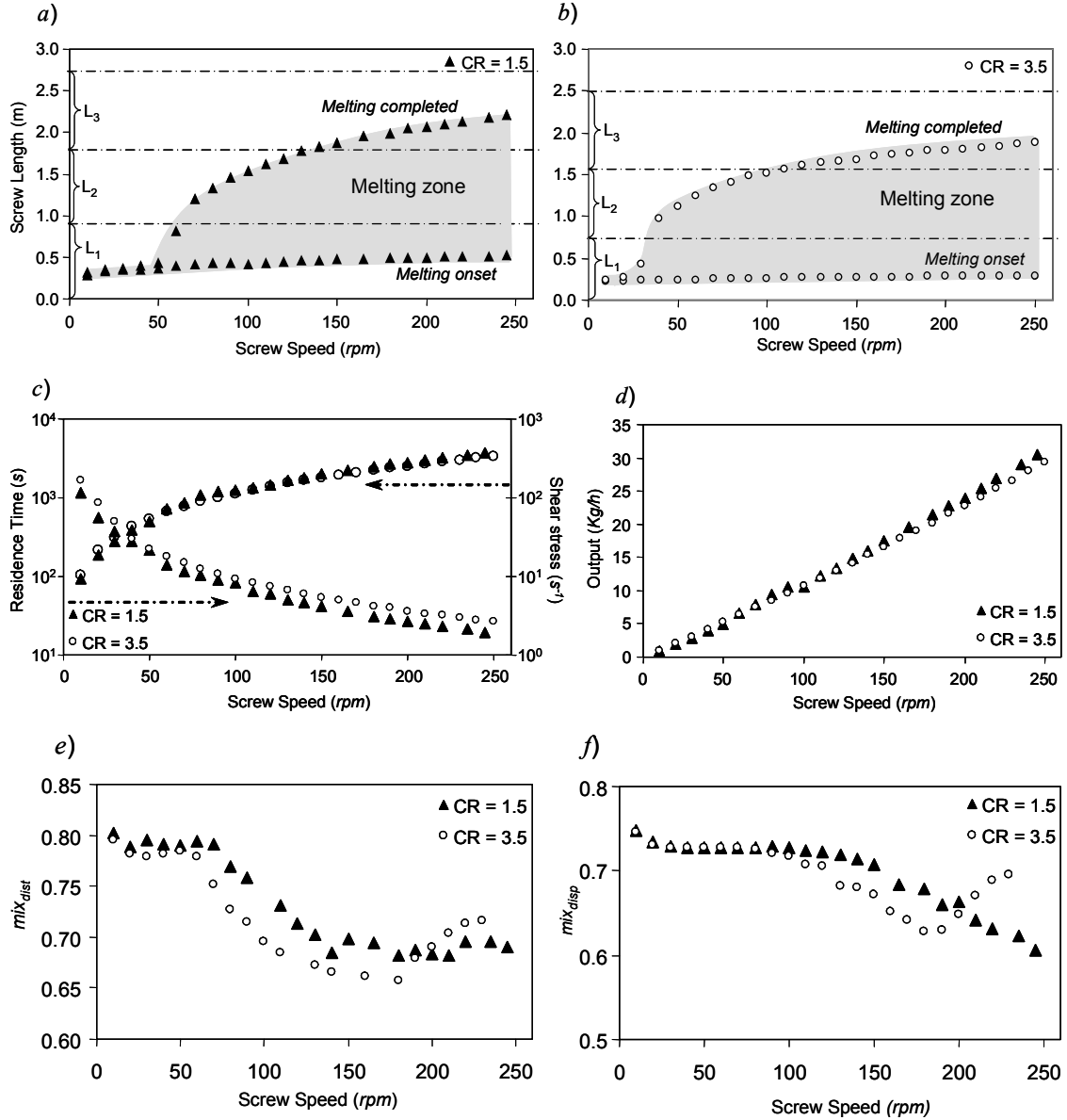


Figure 4: Effect of screw speed on the response of two screws with the same size but having different compression ratios. *a)* melting behaviour of screw with smaller compression ratio; *b)* melting behaviour of screw with higher compression ratio; *c)* average shear rate and residence time; *d)* mass output; *e)* global distributive mixing index; *f)* global dispersive mixing index.

Since mass outputs are very similar for both profiles (Figure 4d), average melt shear rates are similar and average melt residence times are slightly higher for the more compressive screw (Figure 4c). The resulting mixing behaviour depicted in Figures 4e and 4f is

complex, showing that, for this particular example, lower compression ratios induce better mixing for low and medium range screw speeds, whereas higher compression ratios become more effective at high screw speeds.

An optimization run using the scale-up methodology was also carried out, with the aim of defining the operating conditions of the target extruder that would induce the same overall mixing behaviour provided by the reference extruder (it was assumed that this was operating with a screw speed of 50 rpm and a flat barrel temperature of 190°C). A multi-objective optimization was applied using the two indices simultaneously. The program yielded a few operating windows, where the values of the differences between the mixing indices of the two machines were minimized.

6- CONCLUSIONS

A computational methodology was developed to generate global mixing indices assessing the dispersive and distributive mixing capacities of a given screw. These indices range between 0 and 1, hence they can be easily used for comparing the mixing performance of different geometries processing the same material.

The methodology involves the calculation of the evolution of the size and shape of virtual drops that are considered as suspended in the melt, the pace of insertion matching the melting rate. In other words, mixing is followed from the melting onset until the screw tip, thus encompassing the melting and melt conveying zones. Although not presented here, similar calculations would be possible if solid agglomerates were suspended in the melt [11].

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